NASA-CR-201039

Radiation Effects and Defects in Solids, 1989, Vol. 110, pp. 375–383
Reprints available directly from the publisher
Photocopying permitted by license only

MONTE CARLO CALCULATION OF ELECTRON SPECTRA PRODUCED IN WATER PHANTOMS BY 20 keV–1 GeV PHOTONS

M. L. RUSTGI and L. N. PANDEY

Physics Department, State University of New York, Buffalo, New York 14260

RAM RAJ

Physics Department, Kurukshetra University, Kurukshetra, 132119 India

and

S. A. T. LONG

National Aeronautics and Space Administration, Langley Research Center, Hampton, Virginia 23665-5225

A Monte Carlo calculation for the energy spectra of electrons and positrons produced in infinite and semi-infinite water phantoms by photons ranging in energies from 20 keV to 1 GeV are presented. The dominant processes considered are the photoelectric effect, Auger effect, Compton effect, pair, and triplet production. Bremsstrahlung produced by electrons and positrons with energies greater than 1 MeV is also included. The effect of multiple Compton scattering, not considered in the earlier calculation, for the infinite phantom for photon energies higher than 2 MeV has been incorporated. For a semi-infinite phantom, multiple Compton scattering and backscattering through the top are considered. The results are compared with the earlier calculations for the first-collision spectrum. It is found that the inclusion of multiple Compton scattering significantly increases the average number of electrons/cm^3 per photon/cm^2 at all energies considered whereas bremsstrahlung reduces the number of high energy electrons and produces more low energy electrons in the spectrum.

Key words: electron spectra, photon irradiation, water phantoms, Monte Carlo simulation, high energy photon effects.

1 INTRODUCTION

When a low-energy photon enters a medium, it is known to alter the properties of that medium through the photoelectric and Compton effect. At higher energies, pair and triplet production become increasingly important. The threshold for pair production is 1.022 MeV and for triplet production it is four times the rest mass of an electron. Electrons and positrons produced by photons in pair and triplet production can cause further damage to the water molecules.

In our earlier paper,[1] initial electron energy spectra produced in semi-infinite and finite water phantoms irradiated by photons of energies up to 2 MeV was presented. Because of the low energy of the photons only photoelectric effect, Auger effect, and multiple Compton scattering were included. In the present paper these calculations are extended to 1 GeV and pair and triplet production along with bremsstrahlung or radiative collisions by electrons and positrons of energies greater than 1 MeV are also included. The electron interaction with bound electrons is not included and will be the subject of a future investigation. Moreover, the results are presented in units such that kerma in water can be calculated from the table values.

2 NUMERICAL CALCULATIONS

As mentioned earlier, a photon impinging upon a material can produce electrons through Compton scattering and photoelectric effect and electrons and positron through pair and triplet production depending upon the incident photon energy. High energy electrons and positrons can suffer radiative collisions and produce bremsstrahlung and these photons in turn produce more electrons.

The production of Compton electrons, photoelectrons and Auger electrons have been already discussed in our earlier paper.[1] However, Auger effect followed by Compton scattering not considered before is also included here. This will result in an increase in the number of electrons in the lowest energy interval. For calculations, photon cross sections for various processes at different photon energies are taken from the tables of Hubbel[2] and Hubbel *et al.*[3]

Energy distributions of electrons and positrons produced by pair production in the field of a nucleus has been calculated employing the formulas given by Bethe and Ashkin.[4] The cross section given by Bethe and Ashkin[4] is evaluated and plotted by choosing the ordinate in such a way that for a particular photon energy, the area under the curve for the cross section versus the kinetic energy of positron (electron) in units of total available kinetic energy yields the total cross section for the creation of a positron (electron). The kinetic energy T_P of a positron produced in a pair by a photon of energy k can be calculated with the help of a random number and the ratio of the areas under the curve from 0 to T_P and from 0 to T_{max} ($= k - 2\mu$, μ is electron rest mass). The kinetic energy T_E of the electron in the pair, hence, will be $k - 2\mu - T_P$. The energy distribution of pairs produced in the field of an atomic electron is assumed to be the same as that for the pair in the field of a nucleus. The energy of the triplet "target" electron has been calculated by an approximate formula for the momentum distribution given by Bethe and Ashkin.[4] The percentage contribution of pair and triplet production to the total cross-section at 1 GeV is 45 and 49% for H and 86 and 12% for O, respectively.

It is known that fast electrons and positrons can lose energy in water through collisions or bremsstrahlung or both. In order to make the calculations more tractable, only the bremsstrahlung losses will be included. The collision and bremsstrahlung cross sections are given by Berger and Seltzer[5] and are used to find the probability of bremsstrahlung production. At higher energies, for electrons the dominant way of losing energy is by bremsstahlung production. Since bremsstrahlung contribution is included only for electrons of 1 MeV or higher in energy, photo- and Auger electrons are not treated for bremsstrahlung.

The angular distribution of Compton electrons can be calculated through the kinematics of Compton scattering. The angular distribution of electrons and positrons produced in pair production can be found from the formulas given by Bethe and Ashkin.[4] Once the global positions of electrons and positrons are known, the energy and angular distribution of bremsstrahlung photons are determined by the formulas described by Bethe and Ashkin.[4] These new photons are allowed to produce electrons and positrons in the same way as discussed above. Most of the recoil electrons in triplet production are produced in the 0–1 MeV range and are also not treated for bremsstrahlung.

3 RESULTS AND DISCUSSIONS

Two different phantoms, infinite and semi-infinite, have been considered to calculate the energy distribution of electrons and positrons set in motion in water by the incident monoenergetic photons.

Our first set of calculations for the first-collision spectra without bremsstrahlung is in good agreement with those of Todo *et al.*[6] and only in rough agreement with the results of Cormack and Johns[7] as they did not consider triplet production and did not include Auger electrons followed by Compton scattering. Inclusion of bremsstrahlung decreases the number of high energy electrons and positrons and produces many more low energy electrons and positrons resulting in an increase in the average number of electrons per photon in that range. The electron spectrum below 1 MeV will not be affected due to bremsstrahlung since bremsstrahlung of electrons of energies less than 1 MeV is not considered.

In the earlier paper by Pandey *et al.*[1] only the relative values of the number of electrons/keV per 1000 photons was given. They should be multiplied by the total attenuation coefficient of water in cm^2/gm and density of water in gm/cm^3 to obtain the absolute values in terms of total number of electrons/$cm^3 \cdot keV$ per photon/cm^2 which are convenient to calculate kerma for photons. The values listed in Table I and II of Pandey *et al.*[1] in the lowest energy interval are changed because the contribution of Auger electrons followed by Compton scattering had not been included. The changed values are given in Table I here for photon energies up to 220 keV in the 0–5 keV electron energy interval and in the 0–100 keV interval for 500 and 1000 keV photons.

TABLE I
Initial energy distribution of total number of electrons/cm^3 keV per photon/cm^2. The results of the first collision spectrum are displayed in row (1). The rows marked (2) and (3) represent the results for infinite and semi-infinite phantoms, respectively on including multiple Compton scattering. All the table values are to be multiplied by 10^{-3}

Electron energy interval (keV)		Photon energy (keV)								
			20	30	40	50	60	70	80	90
	(1)		150	75.6	53.8	35.9	28.4	23.6	20.0	17.6
	(2)		221	161	178	186	196	203	205	207
0–5	(3)		185	117	109	95.1	90.8	88.6	85.6	82.9
		100	120	140	160	180	200	220	500*	1000*
	(1)	15.5	12.9	11.1	9.74	8.90	8.18	7.64	0.518	0.241
	(2)	209	209	206	202	198	194	190	15.2	11.2
0–5	(3)	81.3	79.4	77.9	76.0	75.1	73.0	72.8	6.92	5.51

*The numbers are given in 0–100 keV interval.

The calculations considering multiple Compton scattering and bremsstrahlung have been performed for the infinite water phantom and the results are given in Tables II and III for photons of energies ranging from 2 MeV to 1 GeV. For lower energy photons up to 1 MeV one can refer to Tables II and III by Turner *et al.*[8] for the electron energy spectrum except for the lowest energy interval which are given

TABLE II

Energy distribution of total number of electrons and positrons produced in the infinite water phantom for photon energies ranging from 2 to 25 MeV. Number of electrons/$cm^3 \cdot$MeV per photon/cm^2

Electron energy interval (MeV)	Photon energy (MeV) 2	3	4	5	6	7	8	9	10	12	14	16	18	20	22	25
0–1	8877	6956	5806	5016	4426	3981	3608	3318	3087	2751	2461	2256	2091	2000	1891	1766
1–2	352	216	161	134	116	98.4	87.8	79.6	72.4	63.3	56.7	52.2	48.7	46.3	44.1	40.6
2–3		205	126	95.1	77.6	67.7	60.1	55.4	51.5	44.0	40.0	35.7	33.2	30.8	29.6	27.7
3–4			144	87.9	67.7	56.6	50.5	45.3	41.5	35.7	33.7	30.1	28.1	26.2	24.3	22.8
4–5				112	68.9	52.9	45.1	40.4	37.1	31.6	27.5	26.2	25.0	23.0	21.5	20.2
5–6					92.6	55.4	43.6	37.4	33.3	29.3	25.9	23.6	22.0	21.2	20.2	19.0
6–7						79.2	47.4	37.9	33.1	27.5	24.2	21.4	19.8	18.5	18.5	16.4
7–8							68.6	41.6	32.8	25.6	22.5	20.6	19.0	17.5	16.8	16.2
8–9								59.4	36.6	25.9	21.6	19.3	17.9	16.8	15.4	14.5
9–10									53.7	26.2	22.2	19.1	16.9	16.2	15.4	14.1
10–11										30.2	21.8	18.4	16.4	15.1	14.0	13.6
11–12										43.9	21.6	18.4	16.2	14.5	14.4	13.1
12–13											25.0	19.1	16.3	14.1	13.2	12.5
13–14											37.0	18.3	17.1	14.7	13.3	12.3
14–15												21.3	16.2	14.6	13.5	11.8
15–16												32.4	16.5	14.6	13.0	11.3
16–17													18.9	14.3	13.4	11.6
17–18													27.5	15.2	12.5	11.2
18–19														16.4	12.7	11.7
19–20														25.0	13.8	11.1
20–21															15.0	11.3
21–22															21.7	10.9
22–23																11.3
23–24																13.5
24–25																19.1
Average number of electrons/cm^3 per photon/cm^2	0.923	0.734	0.624	0.544	0.484	0.439	0.401	0.372	0.348	0.313	0.284	0.263	0.247	0.238	0.227	0.214

Multiply table values by 10^{-4}

TABLE III
Energy distribution of total number of electrons and positrons produced in the infinite water phantom for photon energies ranging from 30 to 1000 MeV. Number of electrons/$cm^3 \cdot$MeV per photon/cm^2

Electron energy interval (MeV)	Photon energy (MeV)							
	30	50	75	100	250	500	750	1000
0–1	1629	1370	1285	1250	1144	1032	963	894
1–5	25.7	22.0	21.1	20.6	19.2	17.5	16.1	15.2
5–10	14.9	12.5	11.9	11.7	11.1	10.3	9.80	9.10
10–20	10.6	8.94	8.52	8.35	8.03	7.67	7.12	6.71
20–30	10.0	6.83	6.17	6.17	6.04	5.76	5.55	5.18
30–40		5.58	4.83	4.79	4.99	4.78	4.52	4.45
40–50		5.46	4.09	3.98	4.10	4.05	3.97	3.79
50–60			3.62	3.36	3.57	3.44	3.38	3.28
60–70			3.25	2.88	3.02	3.08	2.97	2.92
70–80			1.82	2.62	2.65	2.83	2.75	2.62
80–90				2.32	2.38	2.47	2.44	2.39
90–100				2.36	2.11	2.29	2.26	2.22
100–200					1.32	1.50	1.55	1.55
200–300					0.361	0.780	0.878	0.925
300–400						0.489	0.578	0.625
400–500						0.292	0.391	0.452
500–600							0.280	0.324
600–700							0.180	0.247
700–800							0.0653	0.186
800–900								0.138
900–1,000								0.088
Average number of electrons/cm^3 per photon/cm^2	0.201	0.179	0.175	0.176	0.181	0.182	0.182	0.179

Multiply table values by 10^{-4}

in Table I of this paper. As pointed out earlier, Turner *et al.*[8] did not include Auger electrons which are produced following Compton effect. Due to the inclusion of bremsstrahlung and multiple Compton scattering, the average number of electrons/cm^3 per photon/cm^3 increases by a factor of 16 at 2 MeV and by 4 at 1 GeV when compared with the results of Todo *et al.*[6] In this and the following tables, 25,000 incident photons are considered for each energy to generate the spectrum. For 25 MeV photons, the electron energy spectrum is shown in Figure 1 and compared with the results of Todo *et al.*[6] for the first-collision spectrum. The effect of including bremsstrahlung and multiple Compton scattering is also shown. It is clear from Figure 1 that multiple Compton scattering significantly increases the number of electrons in the lower and middle energy intervals and inclusion of bremsstrahlung on top of that adds more electrons in the lower energy intervals and decreases it in the higher energy intervals.

The results for the energy distributions of electrons and positrons in a semi-infinite water phantom are tabulated in Tables IV and V. The procedure laid down by Pandey *et al.*[1] to incorporate backscattering has been followed. The number of electrons/cm^3 MeV per photon/cm^2 in the lowest energy interval is reduced in

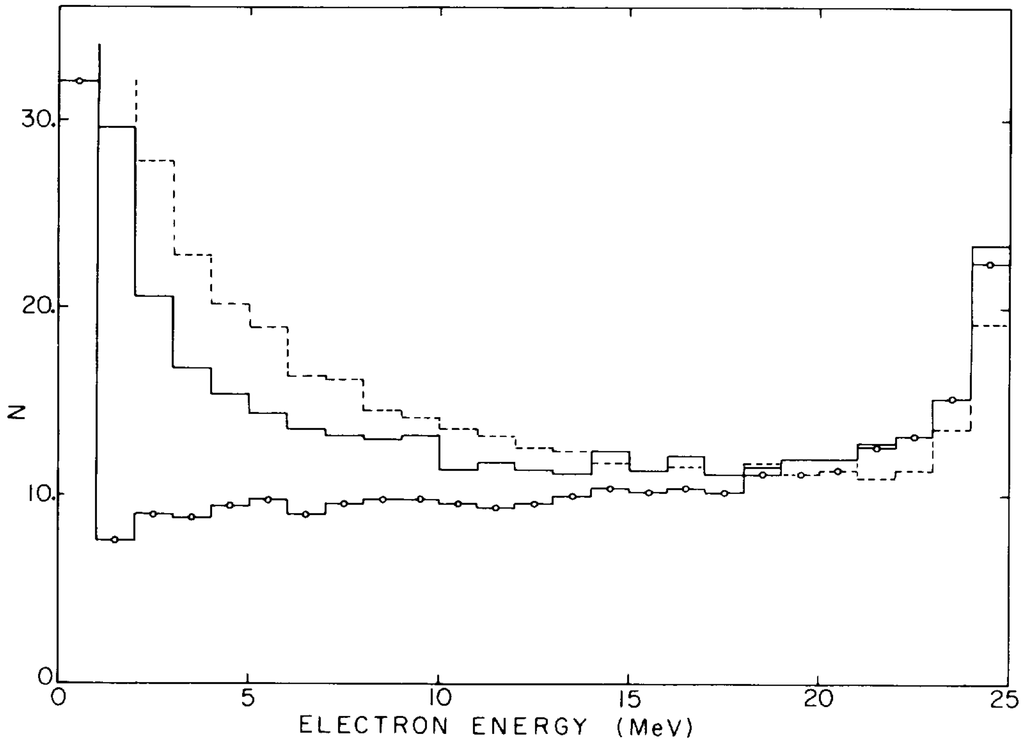

FIGURE 1 Total number (N) of electrons and positrons/cm^3 MeV per photon/cm^2 produced in water by 25 MeV photons as function of electron energy for first-collision (-0- histogram), multiple Compton scattering (solid histogram), and multiple Compton scattering and bremsstrahlung (dashed histogram) in an infinite phantom.

comparison with the results for an infinite phantom because of backscattering. The number of electrons in the second lowest energy interval are a bit higher than the one for the infinite phantom because the electrons in this energy interval arise either from Compton scattering or from pair production and because at low energy they may suffer scattering through angles greater than $\pi/2$. These electrons therefore escape through the top of the phantom. Electrons in the infinite phantom produce bremsstrahlung and move to lower energy intervals. The number of electrons in the higher energy intervals are almost the same and small differences are just statistical. The average number of electrons/cm^3 per photon/cm^2 are less than the corresponding ones for the infinite phantom. A reduction factor (1 − average number of electrons for semi-infinite phantom/average number of electrons for infinite phantom) amounts to 45% at 2 MeV and 3% at 1 GeV. It is clear from the cross sections for the photon absorption processes that the probability to produce a pair of electron and positron increases with photon energy causing a reduction in the number of Compton scatterings. This yields smaller reduction factor at higher energies than at the lower energies. For lower photon energies the electron spectra are given in Table II and III of Pandey et al.[1] but the lowest energy interval values are given here again in Table I because of the inclusion of Auger electrons following Compton scattering.

TABLE IV

Energy distribution of total number of electrons and positrons produced in the semi-infinite water phantom. Number of electrons/cm^3·MeV per photon/cm^3

Electron energy interval (MeV)	Photon energy (MeV)															
	2	3	4	5	6	7	8	9	10	12	14	16	18	20	22	25
0–1	5161	4244	3656	3233	2878	2633	2444	2265	2126	1916	1743	1636	1529	1467	1412	1328
1–2	353	216	161	132	111	98.7	88.4	80.1	73.6	64.7	57.1	53.2	49.5	46.3	44.3	41.2
2–3		206	124	94.0	79.1	67.7	59.1	53.3	50.0	43.1	39.4	35.4	33.0	30.7	29.3	27.8
3–4			146	87.9	66.3	56.7	50.6	45.4	40.6	35.9	32.2	29.3	27.2	25.5	24.7	23.0
4–5				113	67.6	52.4	44.5	39.4	37.8	32.4	28.1	25.8	23.9	23.0	22.1	20.2
5–6					93.9	55.7	44.2	37.6	33.8	29.4	25.5	23.0	21.6	21.2	20.2	19.0
6–7						79.3	47.4	38.7	32.4	27.6	24.2	21.4	19.8	18.8	18.6	16.6
7–8							68.5	41.0	32.8	25.9	22.7	20.9	18.5	18.0	16.7	15.9
8–9								60.3	36.8	26.0	21.7	19.5	18.4	16.4	16.1	15.0
9–10									53.5	27.1	21.6	19.3	17.5	16.4	14.6	14.2
10–11										29.4	22.3	18.4	16.5	15.1	14.6	13.4
11–12										43.2	22.4	18.8	16.2	15.3	14.0	12.9
12–13											24.6	18.5	16.4	14.7	13.9	12.4
13–14											36.8	19.1	15.9	14.7	13.4	11.9
14–15												21.2	15.6	14.3	13.5	11.9
15–16												32.1	16.8	14.0	12.9	11.8
16–17													19.3	13.9	12.5	11.4
17–18–													28.3	14.6	12.2	11.3
18–19														16.9	12.4	11.4
19–20														25.1	13.0	10.8
20–21															15.4	11.6
21–22															22.7	10.5
22–23																11.7
23–24																13.2
24–25																19.3
Average number of electrons/cm^3 per photon/cm^2	0.551	0.467	0.409	0.366	0.330	0.304	0.285	0.266	0.252	0.230	0.212	0.201	0.190	0.184	0.179	0.171

Multiply table values by 10^{-4}

TABLE V
Energy distribution of total number of electrons and positrons produced in an infinite water phantom for photon energies ranging from 30 to 1000 MeV. Number of electrons/cm^3·MeV per photon/cm^2

Electron energy interval (MeV)	Photon energy (MeV)							
	30	50	75	100	250	500	750	1000
0–1	1255	1119	1093	1071	1039	969	910	840
1–5	25.8	21.5	20.8	20.2	19.0	17.4	16.2	15.2
5–10	14.9	12.5	11.9	11.7	11.0	10.2	9.84	9.03
10–20	10.7	8.90	8.46	8.30	8.07	7.67	7.09	6.73
20–30	10.0	6.69	6.09	6.10	6.06	5.75	5.45	5.18
30–40		5.61	4.80	4.75	4.96	4.83	4.42	4.45
40–50		5.55	4.13	3.94	4.08	4.01	3.97	3.84
50–60			3.60	3.29	3.52	3.53	3.39	3.27
60–70			1.87	2.96	3.10	3.10	3.01	2.99
70–80			1.82	2.58	2.64	2.83	2.74	2.59
80–90				2.38	2.38	2.46	2.51	2.41
90–100				2.35	2.12	2.29	2.30	2.18
100–200					1.31	1.50	1.55	1.55
200–300					0.362	0.795	0.885	0.921
300–400						0.487	0.575	0.619
400–500						0.287	0.394	0.453
500–600							0.275	0.325
600–700							0.182	0.251
700–800							0.0646	0.186
800–900								0.138
900–1,000								0.893
Average number of electrons/cm^3 per photon/cm^2	0.164	0.153	0.156	0.158	0.171	0.176	0.177	0.174

Multiply table values by 10^{-4}

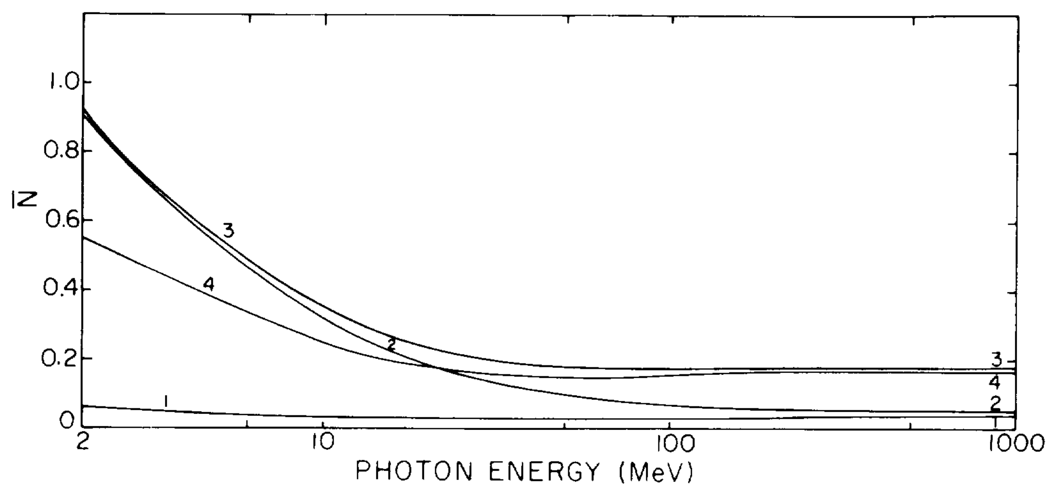

FIGURE 2 Average number ($\bar{N}$) of electrons and positrons/cm^3 per photon/cm^2 versus photon incident energy. The curve marked 1 shows the result for first-collision while other curves 2–4 incorporate multiple Compton scattering, multiple Compton scattering and bremsstrahlung in infinite phantom, and backscattering as well in semi-infinite phantom, respectively.

Figure 2 shows the average number ($\bar{N}$) of electrons/cm^3 per photon/cm^2 versus photon incident energies from 2 MeV to 1 GeV for different calculations performed here. The large reduction in $\bar{N}$ up to 20 MeV as observed in going from curve 3 to curve 4 is mostly due to backscattering of photons because the probability for pair production is not high up to that energy. However, at higher energies the two phantoms, with bremsstrahlung, yields almost the same value of $\bar{N}$ because photon backscattering becomes less prominent.

In conclusion, we have presented a Monte Carlo calculation for energy distributions of electrons and positrons produced in infinite and semi-infinite water phantoms by photons of energies ranging from 20 keV to 1 GeV and found that inclusion of multiple Compton scattering significantly increases the number of electrons over the first-collision spectrum in an infinite phantom. The effect of backscattering in a semi-infinite phantom is found to be mostly important up to about 30 MeV. The inclusion of bremsstrahlung reduces the number of high energy electrons and increases the lower energy ones.

A detailed calculation incorporating multiple Compton scattering, bremsstrahlung production, position annihilation in flight, Møller and Bhabha scattering from electrons and Molière multiple scattering from atomic nuclei has been completed and will be soon published.

ACKNOWLEDGEMENT

This work was partially supported by the National Aeronautics and Space Administration under Grant No. NAG1577.

REFERENCES

1. L. N. Pandey, M. L. Rustgi, and S. A. T. Long, *Health Phys.*, **53**, 163 (1987).
2. J. H. Hubbel, "Photon cross section, attenuation coefficients, and energy absorption coefficients from 10 keV to 100 GeV", National Standard Reference Data Series, National Bureau of Standards, No. 29, (Washington, D.C., 1969).
3. J. H. Hubbel, H. A. Gimm, and I. Overbo, *J. Phys. Chem. Ref. Data*, **9**, 1023 (1980).
4. H. A. Bethe and J. Ashkin, Passage of radiation through matter, in *Experimental Nuclear Physics*, E. Segrè (Ed.), Vol. I (New York, Wiley, 1953).
5. M. J. Berger and S. M. Seltzer, "Tables of energy losses and range of electrons and positrons", Studies in Penetration of Charged Particles in Matter, National Academy of Science-National Research Council, publication 1133 (Washington, D.C., 1964).
6. A. S. Todo, G. Hiromoto, J. E. Turner, R. N. Hamm, and H. A. Wright, *Health Phys.* **43**, 845 (1982).
7. D. V. Cormack and H. E. Johns, *Br. J. Radiol.* **25**, 369 (1952).
8. J. E. Turner, R. N. Hamm, H. A. Wright, J. T. Modolo, and G.M.A.A. Sordi, *Health Phys.* **39**, 49 (1980).